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Headquarters U.S. Air Force

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Design of Experiments (DOE) for Validation of STORM Based on THUNDER



**73rd MORSS, USMA 2005
WG 25 & 29**

**Mr. Tom Chwastyk
AFSAA/SAAT**

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Purpose

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- THUNDER vs. STORM
- Goal of DOE here: V&V by comprehensive comparison
 - Why not VV&A?
- General and specific models of the V&V experiment
- DOE for adequate excitation to compare responses
 - Screening to reduce response model size
 - Adding design points to check for interactions
- Comparing THUNDER and STORM response
 - By Singular Value Decomposition
 - By Canonical Correlation
- Automating execution of runs and extraction of results
 - Work in progress – all feedback welcome
- Punch line: Massive quantitative validation experiment – uses computers and sophisticated techniques to exceed past human limits on data production and interpretation

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THUNDER vs. STORM

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■ THUNDER: accepted standard

■ Not Government owned

■ Proprietary engine, SIMSCRIPT

- CACI licenses – big \$\$\$ / seat / year

■ Ground war:

- “Pistons” define FLOT
- Piston walls do not reorient as FLOT distorts

■ No study manager -- manual file configuration control

■ Minimal GUI

■ Minimal ISR

■ STORM: AFSAA’s next standard

■ Government owned

■ Open source, non-proprietary

- Simulation engine in g++ ; maps, DB tools; even OS, all open
- No per-seat license fees

■ Ground war:

- Along arcs and within nodes
- Shape of FLOT morphs naturally under network constraints

■ Study manager automates file configuration control

■ Extensive GUI – map tool, report tool, graph tool

■ Sat tool and other significant ISR developments

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V&V by Comparison (Not VV&A?)

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■ V&V

■ Verification: “Solve the Problem Right”

- Identify and fix lurking code problems

■ Validation: “Solve the Right Problem”

- Accepted referent is THUNDER but comparison is a hard problem

■ Comparison needed over a set of scenarios of interest

- Are results “comparable to or better than” THUNDER? Just what does that mean?
 - SME’s “face validation” vs. statistical tools – both are needed
- Does DOE show effects of changes in STORM vs. THUNDER?

■ Why V&V, not VV&A?

■ A (Accreditation) is PM’s decision – balancing risk versus resources

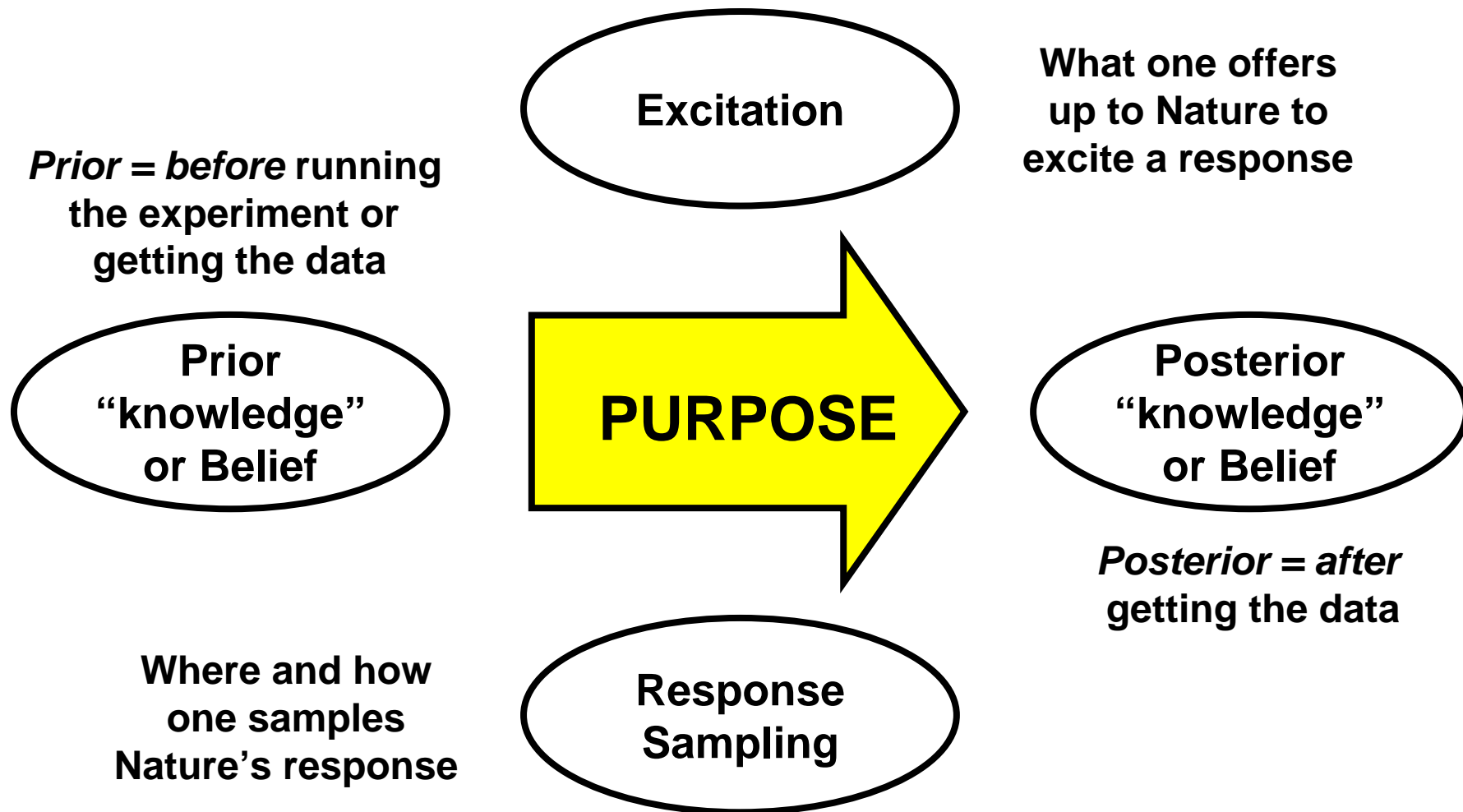
- Too little V&V: low resource expenditure but high risk
- Too much V&V: little risk reduction for last expenditures



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A General Model of an Experiment

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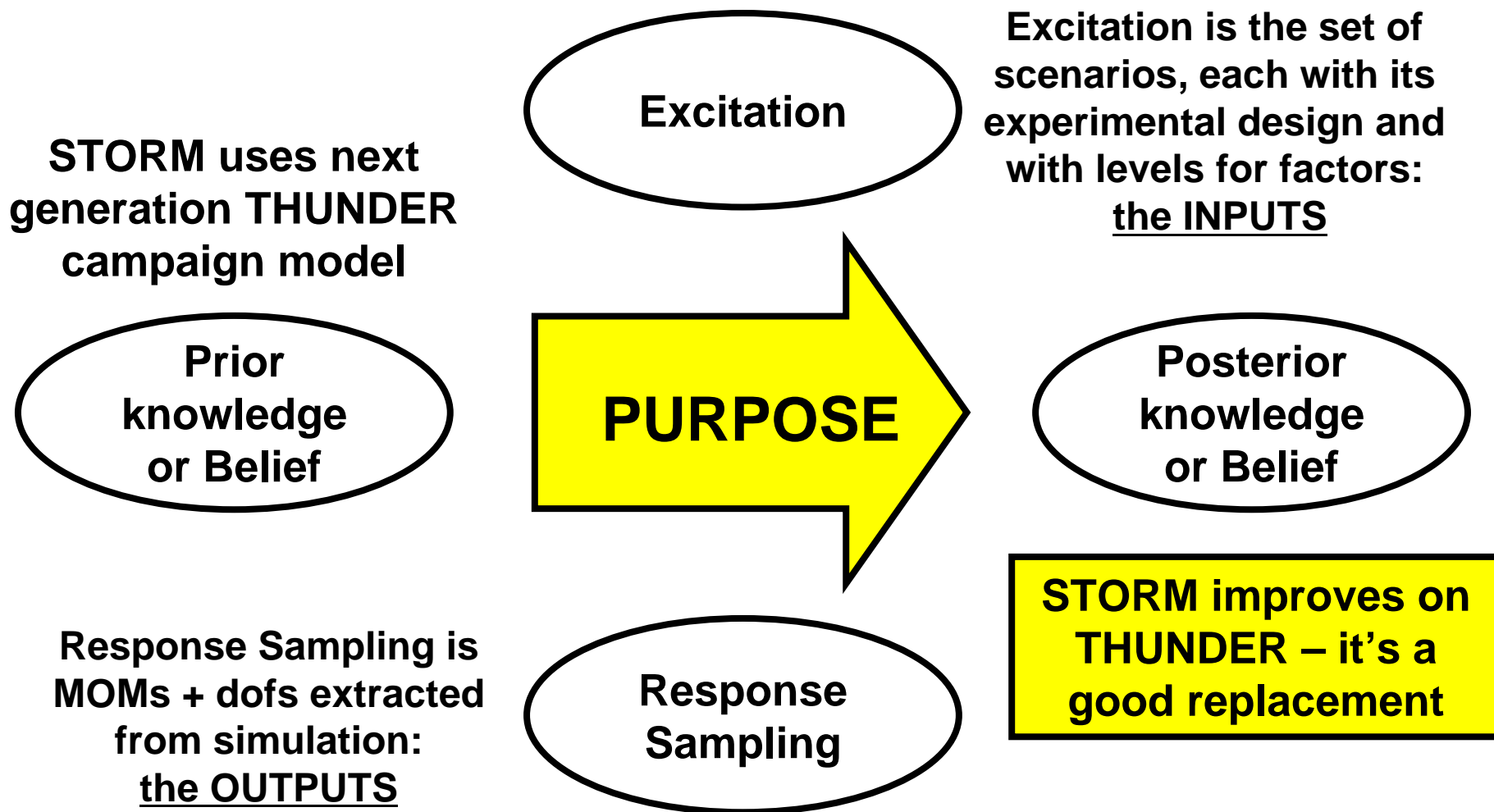




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...Tailored to V&V and Comparison

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V&V Scenario Set of Interest

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- Consult with SMEs, see for what campaign models/scenarios THUNDER results (inputs and outputs) are already available and of interest
 - THUNDER has been much more expensive to run (small error \Rightarrow typically 60-100 reps) than STORM – hence, minimize additional THUNDER runs
- Choose among available THUNDER campaigns to agree on sufficiently complete V&V scenario set
- If necessary, add THUNDER or STORM work to achieve common and complete set of scenarios of significant interest for V&V



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Need to Reduce Input Dimensions

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- | | | | |
|---------|------|-----|-----------------------------|
| THUNDER | v6.9 | 99 | *.dat files |
| STORM | v1.3 | 115 | *.dat files (plus path.dat) |
- Typical .dat file has 10 to 1000+ parameters (inputs) – highly interrelated, often nonlinearly
- Too many parameters to screen individually
 - Use SME's to combine (cull?) inputs into fewer (10 to 100) factors $f_i \equiv_{\text{def}} [p_{i,j}]$ parameter vectors
 - $p_{i,j}$, $p_{i,k \neq j}$ need not be in same .dat file
 - Each parameter in a factor has two levels, A / B – goes A / B as its factor goes high / low – no “within-factor interactions”
- Factor screening takes place in STORM across entire V&V scenario set at once
- Whether the change in level of factor f_i is significant depends both on the scenario set and on what MOM(s) or output dof(s) are of interest

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Input Sensitivity Screening

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- Initial screening in STORM of two-level factors
 - Resolution V (preferred) or IV (if necessary) fractional factorial (FF) – possibly even res. III for initial stab?
 - If resolution IV necessary, follow up with resolution V (res. IV significant factors only, plus all 2-factor interactions) to screen for significant interactions
 - 256 reps (resolution IV) \Rightarrow up to 128 factors
 - Comparable to # of reps in STORM V&V reports for previous releases (19 + cases x 10 repeated reps / case)
 - Likely fewer factors (≤ 64 , ≤ 32) if long reps ($t_{sim} \gg 10$ days)
 - However, 256 reps (resolution V) \Rightarrow
only 12 to 17 factors (+ all 2-level interactions)
- In any case –
 - NOT One-Factor-At-a-Time as before!
 - NO replicated design points (reps)!

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Matrix Model Equations

$$\mathbf{Y} = \mathbf{XB} + \mathbf{E}$$

$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\mathbf{B}} + \hat{\mathbf{E}}(\mathbf{s})$$

$$\hat{\mathbf{E}}'_i = \left[f_1(s_i) \cdots f_j(s_i) \cdots f_m(s_i) \right]'$$

$\hat{\mathbf{B}}$ is by least squares, minimizes

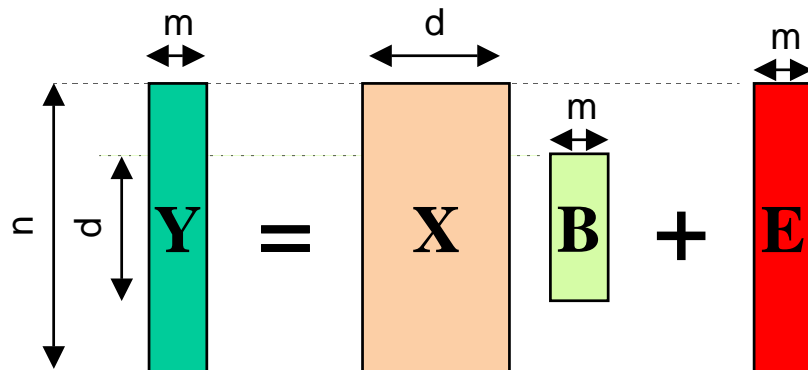
$$RSS = \sum_i \sum_j (y_{ij} - \hat{y}_{ij})^2$$



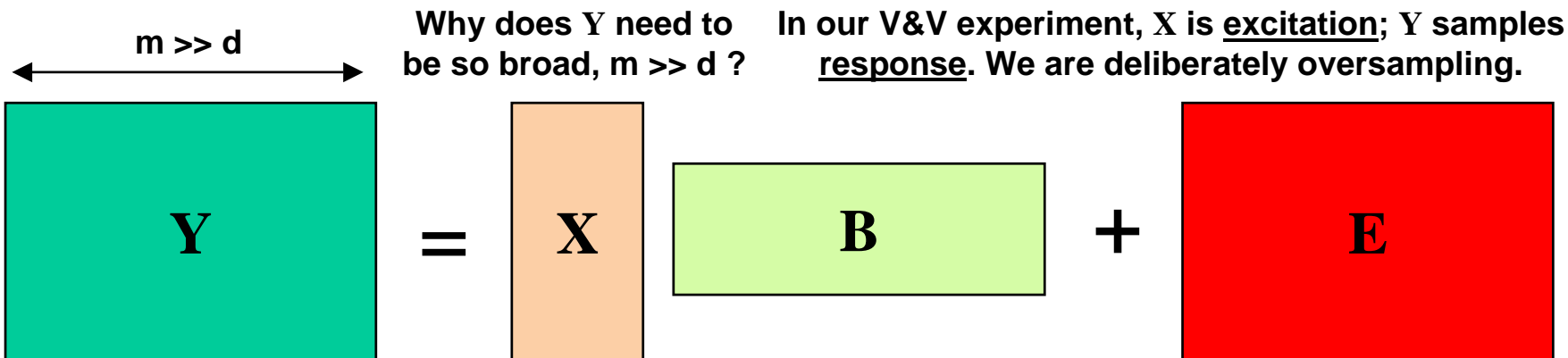
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Not Your Usual Few Responses

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m = # of response variables
 d = # of design variables (factors)
 n = # of runs
 $n > d$ (always)
 $m \ll d$ (usually)



We oversample by several times the dimensionality of our excitation in a “shotgun approach”, hoping we catch most of the significant dimensions of model response.

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Why Fit Is Always Too Good

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$$Y = X B + E$$

$$\hat{Y} = X \hat{B} + \hat{E}$$

$$X' E \neq 0 = X' \hat{E}$$

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Elements of Matrix Model

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- Starts as typical multivariate response model
 - Response matrix Y ($n \times m$)
 - Design matrix X ($n \times d$)
 - Effects matrix B ($d \times m$)
 - “Out-of-model” matrix E ($n \times m$)
 - Estimates “hatted”: \hat{E}, \hat{B}
- Beyond typical model:
 - *Compute* Y from X in permuted order $pc^{(1)}, pc^{(2)}, pc^{(3)}$, but *record* Y in design order (picture of $Y, pc_{i}, pc^{(i)}$ later)
 - Record random seed and permuted computational order $[s_i \ pc_{i}]$ for row i ($n \times 2$)



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Design Matrix X - Words

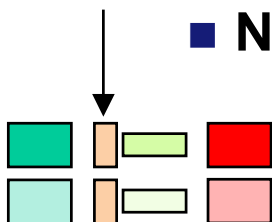
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■ ROWS in the design matrix X

- Give particular combination of factor levels for each design point
- Cover all scenarios of interest
- Contain a non-zero entry in only one of the columns indicating scenarios

■ COLUMNS in the design matrix X

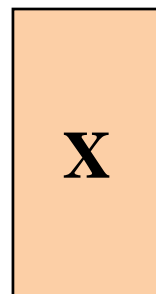
- Signify design (input) factors
- Signify scenarios for estimating mean
 - Decompose sum of squares due to scenario means
 - Number of means is included in d, # of design variables





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scenario #	1	2	3	4	5	6	7	8	9	10	factor level
------------	---	---	---	---	---	---	---	---	---	----	--------------

1	0	0	0	1	3	5	7	2	8
1	0	0	0	2	4	6	7	2	8
1	0	0	0	2	4	5	7	2	8
1	0	0	0	1	3	6	7	2	8
0	1	0	0	1	3	5	8	7	1
0	1	0	0	2	4	6	8	7	1
0	1	0	0	2	4	5	8	7	1
0	1	0	0	1	3	6	8	7	1
0	0	1	0	1	3	6	8	7	8
0	0	1	0	1	3	5	8	2	1
0	0	1	0	1	3	6	7	7	8
0	0	1	0	1	4	5	7	2	1
0	0	1	0	1	4	6	8	7	8
0	0	1	0	1	4	5	7	2	1
0	0	0	1	1	4	6	8	2	8
0	0	0	1	2	3	6	7	2	8
0	0	0	1	1	3	6	8	2	1
0	0	0	1	2	3	5	7	7	1
0	0	0	1	1	3	5	7	7	8
0	0	0	1	2	4	5	8	7	8

constant factor level
within scenario says
significance of
factor is not tested
within scenario

1's account for
scenario means, ssq

Notional design
only, not 2^{k-p}

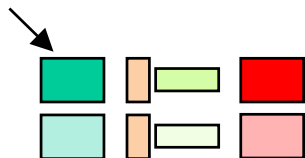


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Response Matrix Y - Words

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- **ROWS** in the response matrix Y
 - Correspond to design matrix rows
- **COLUMNS** in the response matrix Y signify
 - Scalar or vector MOMs / dofs
 - Consistent responses for each row and scenario
 - Squadrons or other entity types handled differently by planning files on different design points should not re-use the same response columns unless
 - the difference in response due to difference in planning file parameters is the effect being sought and
 - the difference in planning file parameters is reflected in one or more factors



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Response Matrix - Picture

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pco (i)	pco _i	scenario #	i = row # in X	Scalar MOM 1	Scalar MOM 2	Scalar MOM 3	Vector dof 1 day 1	Vector dof 1 day 2	Vector dof 1 day 3	...	Vector dof 1 day n-1	Vector dof 1 day n	Scalar MOM 4	Vector dof 2 day 1	Vector dof 2 day 2	Vector dof 2 day 3	...	Vector dof 2 day n-1	Vector dof 2 day n	Scalar MOM 5	Vector dof 3 day 1	Vector dof 3 day 2	...	Vector dof 3 day n-1	Vector dof 3 day n	Vector dof 4 day 1	...	etc.
13	14	1	1																									
11	3	1	2																									
2	5	1	3																									
7	9	1	4																									
3	11	2	5																									
10	12	2	6																									
12	4	2	7																									
8	8	2	8																									
4	13	3	9																									
14	6	3	10																									
5	2	3	11																									
6	7	3	12																									
9	1	3	13																									
1	10	4	14																									
...																									

Y

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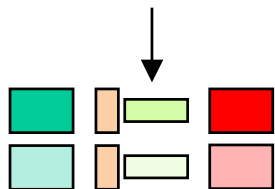


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Effects Matrix B, B hat

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- **ROWS** in the effects matrix B
 - Correspond to design variables
 - For SME-aggregated factors, coefficient shows effect of change in level
 - For scenario indicator variables, coefficient shows scenario mean for each response
- **COLUMNS** in the effects matrix B
 - Correspond to response MOMs, dofs



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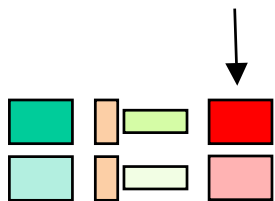


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Out-of-Model Matrix E , E hat

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- Part of E is assumed due to stochastic effects
 - Neither random seed value s_i nor its effect $f_j(s_i)$ on each response y_{ij} is known to the fitting process
 - s_i and $f_j(\bullet)$ —hence $f_j(s_i)$ —are termed exogenous (excluded from model)
- Effects of exogenous variables, *including stochastic effects*, alias to an unknown extent onto endogenous (included in model) effects b_j



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Interactions, Response Surface

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- Once factors and 2-factor interactions are identified as significant at resolution V, high-low level only ...
- Add intermediate levels as appropriate to gain Response Surface Model (RSM)
 - Central composite design if appropriate
- Retain only statistically significant factors (and interactions) for comparing STORM to THUNDER
 - Not normal statistical practice to “cherry pick” interactions without physical model justification
 - Empirically justifiable because RSM is descriptive only, not first principles
 - We are a long way off from this

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Dimension Reduction (1): RSM

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- Add face and center points for significant factors to get central composite design if feasible
- Possibly use intermediate points for near-orthonormal Latin Square
- Get response surface model (RSM) – polynomial or spline
 - Stop on Mallow's C_p or other measure of complexity vs. goodness of fit
- Retains coordinates of original model space

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Weight Questions (1)

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- **Question 1: What is the proper weight or scale per MOM / dof(s) in the penalty function for lack of fit?**
 - That is, how much should lack of fit in one column (or set of columns) of Y count relative to lack of fit in another column (or set of columns)?
- **Question 2: Same as Question 1 but for one scenario (set of rows) versus another**



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Weight Answers (Partial) (2)

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- **Depends on user goal and on STORM / THUNDER comparison approach**
 - **Data for SVD, canonical correlation should have zero scenario mean**
 - **Appears no natural scale for Singular Value Decomposition (SVD); use unit column variance for consistency with canonical correlation**
 - **Scale set to unit column variance by definition of canonical correlation, but meaning and appropriateness to user goal are not clear**
 - **Beware augury / mysticism / wise chin-scratching**



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Equations in Passing

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- Final dry run for this brief commented that there were way too many equations, too few graphics
- Graphics proved far more time consuming to produce than initially expected
- Equations were retained more as art objects and speaking totems than as detailed communication tools
- Equations past the basic “Matrix Model Equations” will not be on the midterm or the final



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Dim. Red. (2): SVD (1)

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- Singular Value Decomposition (SVD) on responses Y adjusted to zero-scenario-mean, scaled to unit Y column norm, and transposed*:

* not a good idea, but not fatal

$$\mathbf{Y}_{zsm} = \mathbf{Y}(\mathbf{I}_n - \underbrace{\mathbf{X}_{sm}(\mathbf{X}_{sm}'\mathbf{X}_{sm})^{-1}\mathbf{X}_{sm}'}_{\mathbf{X}_{sm} = \text{only columns for scenario means}})$$

$\mathbf{X}_{sm} = \text{only columns for scenario means}$

$$\mathbf{A}_{(m \times n)} = (\hat{\mathbf{Y}}_{zsm})', (\hat{y}_{zsm})_{ij} = (y_{zsm})_{ij} / \sqrt{\sum_{i'=1}^n (y_{zsm})_{i'j}^2}$$

$$\mathbf{A} = \mathbf{O}\mathbf{D}\mathbf{V}' \begin{cases} \mathbf{O}'\mathbf{O} = \mathbf{I}_n, (m > n) \Rightarrow \mathbf{O}\mathbf{O}' \neq \mathbf{I}_m \\ \mathbf{D} \text{ diagonal, p.s.d., } (i < j) \Rightarrow (d_{ii} \geq d_{jj}) \\ \mathbf{V}\mathbf{V}' = \mathbf{V}'\mathbf{V} = \mathbf{I}_n \end{cases}$$



■ Continuing,

$$\mathbf{A}'\mathbf{A} = \mathbf{Z} = \mathbf{V}\mathbf{D}'\mathbf{O}'\mathbf{O}\mathbf{D}\mathbf{V}'$$
$$= \mathbf{V}\mathbf{D}^2\mathbf{V}'$$

$$\mathbf{Z}\mathbf{V} = \mathbf{V}\mathbf{D}^2\mathbf{V}'\mathbf{V} = \mathbf{V}\mathbf{D}^2$$

$$\mathbf{Z}\mathbf{V} = \mathbf{V}\mathbf{\Lambda} \quad (\text{symmetric eigenproblem})$$

$$d_{ii} = \sqrt{\lambda_i} \quad (\text{sorted } \lambda_1 \geq \lambda_2 \geq \dots \lambda_n \geq 0)$$

$$\mathbf{O}_i = \mathbf{A}\mathbf{V}_i d_{ii}^{-1} \quad \text{canonical column } i \text{ of } \mathbf{A} \text{ for } d_{ii} > 0$$

■ Why is this significant?



... SVD (3)

- This is significant *because...*

$$\mathbf{A} = \mathbf{O}\mathbf{D}\mathbf{V}' = \sum d_{ii} \mathbf{O}\mathbf{V}' \text{ (exactly!) and}$$

$$\sum_j \sum_k (\mathbf{O}_i \mathbf{V}_i')_{jk}^2 = \sum_j \sum_k (o_{ji} v_{ik})^2 = \sum_j o_{ji}^2 \sum_k v_{ik}^2 = 1,$$

so all scale information is in the “singular values” d_{ii} in the sense that d_{ii}^2 shows how many unit rows of \mathbf{A} are expressed by $d_{ii} \mathbf{V}_i'$.

- This means that the completeness $R^2(k, m)$ of expressing all m unit rows of the response matrix \mathbf{A} using only k coefficients is

$$R_{k,m}^2 = \left(\sum_{i=1}^k d_{ii}^2 \right) / \left(\sum_{i'=1}^m d_{i'i'}^2 \right)$$

- More on SVD follows after discussion on Canonical Correlation



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DR (3): Canonical Correlation (1)

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- Two response sets, say $T = \hat{Y}'_T$ for THUNDER and $S = \hat{Y}'_S$ for STORM
- m ROWS of T, S
 - Zero scenario mean, unit variance as for SVD
 - Same row \Leftrightarrow same MOM or dof for T as for S
- n COLUMNS of T, S are in same order as design matrix rows, although design points were computed in permuted sequence(s)



- Canonical correlation (CanCorr) gives $m \times 2$ coefficients $[lca_k \ lcb_k]$ for successive $n \times 2$ linear composites $[u_k \ w_k]$, such that for $u_k' = lca_k' T$, $w_k' = lcb_k' S$, $k = 1, 2, \dots, \min(m, n)$
 - u_k and w_k have maximal correlation ρ_k^* between any two linear composites of T, S not spanned by $[u_1 \ u_2 \ \dots \ u_{k-1}]'$, $[w_1 \ w_2 \ \dots \ w_{k-1}]'$
 - $\text{Var}(u_k) = \text{Var}(w_k) = 1$
 - $\rho_1^* \geq \rho_2^* \geq \rho_3^* \geq \dots \rho_{\min(m, n)}^* \geq 0$
 - For $j > k$, u_j and w_k are uncorrelated, i.e.,

$$u_j' (I - 1(1'1)^{-1}1') w_k = 0$$



- How does this work? From the zero scenario means, unit row norms, and definition of variance we get

$$\mathbf{0}_{(2m \times 1)} = \begin{bmatrix} \mathbf{T} \\ \mathbf{S} \end{bmatrix} \mathbf{1}_{(n \times 1)}$$

$$\mathbf{\Sigma}_{(2m \times 2m)} = \frac{1}{n - n_{zsm}} \begin{bmatrix} \mathbf{T} \\ \mathbf{S} \end{bmatrix} \begin{bmatrix} \mathbf{T} \\ \mathbf{S} \end{bmatrix}'$$

$$= \begin{pmatrix} \mathbf{\Sigma}_{TT} & \mathbf{\Sigma}_{TS} \\ \mathbf{\Sigma}_{ST} & \mathbf{\Sigma}_{SS} \end{pmatrix} = \begin{pmatrix} \mathbf{\Sigma}_{11} & \mathbf{\Sigma}_{12} \\ \mathbf{\Sigma}_{21} & \mathbf{\Sigma}_{22} \end{pmatrix}$$



- Then it can be shown in about 3 textbook pages that

$$\begin{bmatrix} \mathbf{u}_k \\ \mathbf{w}_k \end{bmatrix} = \begin{bmatrix} \underbrace{\mathbf{e}_k' \Sigma_{11}^{-1/2} \mathbf{T}}_{\text{lca}_k} \\ \underbrace{\mathbf{f}_k' \Sigma_{22}^{-1/2} \mathbf{S}}_{\text{lcb}_k} \end{bmatrix}, \text{ where}$$

$\text{Corr}(\mathbf{u}_k, \mathbf{w}_k) = \rho_k^*$ is the k^{th} largest eigenvalue of

$$\Sigma_{11}^{-1/2} \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \Sigma_{11}^{-1/2}, \text{ with eigenvector } \mathbf{e}_k, \text{ and also of}$$

$$\Sigma_{22}^{-1/2} \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} \Sigma_{22}^{-1/2}, \text{ with eigenvector } \mathbf{f}_k.$$



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... CanCorr (5)

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- First approach will be to look at initial canonical variables (cv's) as long as ρ_k are well separated
 - If ρ_k are closely spaced, eigenvectors and hence cv's are determined only up to rotations
- Second approach will be to look at residuals once projections on all cv's from 1 to k are removed, for k's such that
 - k is not in the middle of a closely spaced block of ρ_k
 - k is not so far beyond 1 that any patterns apparent in residuals are as likely to be artifacts of numerical methods as of remaining THUNDER vs. STORM relationships
- We have not done this before; any advice would be welcome.

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SVD versus CanCorr: SVD (4)

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- $\mathbf{A}'\mathbf{A} = \mathbf{Z}$ of the SVD development can now be seen as Σ_{22} of CanCorr.
- We also have Σ_{12} , the covariation of T with S. We can estimate what we would expect for T based on S using the first k singular vectors of S as

$$\hat{\mathbf{T}}(\mathbf{S}, k) = \Sigma_{12}(\Sigma_{22})^{-1|k} = \Sigma_{12}\mathbf{O} \begin{pmatrix} d_{11}^{-1} & 0 & \dots \\ 0 & \ddots & \\ \vdots & & d_{kk}^{-1} \\ & & & 0 \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix} \mathbf{O}'$$

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SVD versus CanCorr: SVD (5)

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- **Similar remarks and approaches as for CanCorr apply to SVD**
 - **Singular vectors are less well defined as eigenvalues become closely spaced**
 - **We may look at the fits (estimated values) first if most of the significance falls into a few numerically stable patterns**
 - **We will look at residuals as well, particularly at breaks in a block-type pattern of decrease in singular values / eigenvalues**



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SVD versus CanCorr: SVD (6)

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- **The big, big difference between SVD and CanCorr is**
 - **SVD aims to compactly express the variation of a *single* data set**
 - **Covariation with the other data set is dealt with almost as an afterthought.**
- **CanCorr aims to compactly express the covariation of *both* data sets, without favor for one or the other.**



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Automating Runs and Results (1)

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- Again, a work in progress – all feedback welcome
- Number of parameters, factors, runs makes manual DOE setup and execution unattractive for all but small problems
 - Manual "baby steps" on small problems for debugging
- Concept is to factor problem into DOE files giving
 - Design matrix, source citation, permuted computational order
 - Factors and associated parameters, with .DAT file levels for parameters as .DOE factor goes between its levels



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Automating Runs and Results (2)

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- Automate run process
 - Substituting parameter .DAT levels into .DOE files
 - Write result to temporary .DAT files
 - Execute runs in permuted order
- Automate DOE post process
 - Extract results
 - Transfer to statistical software
 - Use stat tools for evaluation and comparison between THUNDER, STORM results on nominally equivalent models



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Punch Line: Quantitative V&V?

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- **This is a massive quantitative validation experiment**
 - **Uses computers to exceed past human limits on data production**
 - **Uses computers and sophisticated math to surpass unaided human limits on data interpretation**
 - **Unexpected differences between THUNDER and STORM will constitute new knowledge**
 - **Finding only differences explainable as due to known deliberate changes would be a disappointment**

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Nothing to Lose But Uncertainty

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- The author's involvement stems from > 20 years trying to compare test data with modeling results
 - 16 years shock testing nuclear powered ships and their components
 - 9 years with robotic test equipment testing composite material systems
 - Assumed material response theory (dissipated energy density) said could account for 60K data points via 125 coefficients and constraints
 - Ability to so compactly model test data gave massive support to underlying theory
- It is long past time for a similar quantitative approach to V&V – and comparing THUNDER and STORM should be a milestone in that effort.

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Questions?

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